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By Ya. B. Zel'dovich and K. I. Shchelkin

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APPLICATION OF PROPAGATION THEORY OF AN ARBITRARY DISCONTINUITY TO CERTAIN CASES OF GAS IGNITION

/Following is the translation of an article by Ya. B. Zel'dovich and K. I. Shchelkin entitled "Prilozheniye teorii rasprostraneniya proizvol'nogo razryva k nekotorym sluchayam vosplameneniya gazov" (English version above) in Zhurnal Eksperimental'noy i teoreticheskoy Fiziki (Journal of Experimental and Theoretical Physics), Vol. 10, No. 5, 1940, pp 569-575./

1. Introduction

The problem of occurrence and propagation of a pressure discontinuity in a gas has a direct application to the theory of occurrence of detonation in gas mixtures. It can have a bearing also in the ignition of certain combustible gases in manufacturing equipment.

In this connection, we develop below the general theory of the propagation of arbitrary discontinuities, and solve two problems which pertain to the aforementioned practical problems.

2. Theory of Propagation of Arbitrary Discontinuity

Let us consider an arbitrary discontinuity in a gas.

Let at the left of the plane A in Fig. 1 the pressure of the gas be P, the specific volume V, and the molecular weight M. On the right the corresponding values are P_0, V_0, and M_0. The velocity of the gas of the motion is U and U_0 respectively.

What takes place in such a discontinuity?

We call attention to the fact that the change in all the values which describe the gases on both sides of the plane A will henceforth depend only on the ratio x/t, where x is the distance from the point of formation of the discontinuity and t is the time from the instant of its occurrence. This follows from dimensionality considerations. In fact, from the values of P, V, and U we can obtain the length and the time only in the form of a combination of x/t, which represents some characteristic value of the dimension of length. An example of such a quantity is the velocity of sound, which in gas has a value $C = \sqrt{kPV}$, where k is the ratio of the specific heats. The dependence of all the values on the ratio x/t indicates that a certain distribution of P, V, and U takes place in space, and ~~kkk~~ all the scales of this distribution will be proportional to the time. Consequently, we shall accomplish our purpose most rapidly by substituting into the equation of hydrodynamics the variable $\xi = x/tc$, so that $\partial/\partial x = (1/t)d/d\xi$, $\partial/\partial t = -(x/t^2)(d/d\xi)$. We obtain

the continuity equation

$$\xi \frac{d\varrho}{d\xi}=\frac{d}{d\xi}\varrho U$$

and the equation of motion

$$(U-\xi)\frac{dU}{d\xi}=\frac{1}{\varrho}\frac{dP}{d\xi}.$$

Integration of these ordinary differential equations which replace for our problem the usual partial differential equations of gas dynamics, leads to the following results in the rarefaction wave. The state of the matter varies along the isentrope (the Poisson adiabat):

$$PV^k = \text{const.} \tag{1}$$

The change in the velocity of motion upon passage of the wave obeys the equation

$$U \pm \frac{2}{k-1}C = \text{const.} \tag{2}$$

The speed of propagation of the given state, which coincides with its coordinate:

$$x/t=\xi=D=U\pm C. \tag{3}$$

The choice of the sign in the formulas is connected with the direction of propagation of the wave (the upper sign for the wave propagating towards increasing x). The velocity of propagation along the rarefaction wave, calculated from formula (3), is a variable quantity. In other words, calculation leads to a finite width of the rarefaction wave, which increases linearly with time:

$$\Delta x=\Delta D t=\frac{k+1}{k-1}\Delta C; \tag{4}$$

The symbol Δ denotes here the difference between the corresponding quantities at the edges of the rarefaction wave, where the jump in the derivative takes place (at points L and M, Fig. 2).

The compression wave cannot be described by Eqs. (1 — 3), which lead in this case to a physically impossible multiply-valued distribution (three values of pressure and density at one and the same point). In this case a discontinuity takes place — a shock wave, in which the state of the matter varies along the Hugoniot abiabat.

$$\tfrac{1}{2}(P+P_0)(V_0-V)=\frac{1}{k-1}(PV-P_0V_0) \tag{5}$$

So that an increase in pressure in the compression wave corresponds to an increase in the entropy; the speed of motion is given by the formula

$$U=\sqrt{(P-P_0)(V_0-V)}. \tag{6}$$

The speed of propagation of the discontinuity

$$D=U_0\pm V_0\sqrt{\frac{P-P_0}{V_0-V}}=U\pm V\sqrt{\frac{P-P_0}{V_0-V}} \tag{7}$$

is greater than the sum of the velocity of sound and the velocity of motion of the gas subject to pressure, but is less than the same sum for the compressed gas. It follows from this equation that two waves cannot propagate in the same direction. This is physically obvious, since all the waves originate in the same place, and at the same time; yet in a gas which is already subject to the action of the wave, any

following wave will travel with a velocity equal to or greater than the velocity of the first wave, so that it is impossible to imagine two waves travelling in the same direction.

A wave propagating in a given gas — whether it be a rarefaction wave or a shock wave — is fully determined by one parameter, for example, the ratio of the densities of the gas before and after the passage of the wave. This parameter already determines all the remaining quantities — pressure, temperature, entropy, speed of motion of the gas after passage of the wave and speed of propagation of the wave — and furthermore in accordance with formulas (1) — (3), if the density decreases (rarefaction wave), or according to formulas (5) — (7) in the case of a compression wave (shock wave). However, in order to describe the behavior of an arbitrary discontinuity, where in addition to the three quantities P, V, and U on one side of the discontinuity there are specified the three values on the other side, it is necessary to have at least three parameters. Yet, as we have seen, two waves can propagate simultaneously in different directions, so that only two parameters are given. We arrive at the necessity for existence of still another discontinuity which, however, must not propagate relative to the gas; in such a discontinuity, which is of a unique kind, the pressures and velocities of motion of a gas should be the same on both sides of the discontinuity; the density, the temperature, and the entropy of the gas are

different on this special discontinuity, and this yields the missing third parameter. In practice, the calculation reduces to choosing such a value of pressure (which is the same on both sides of the special discontinuity, as to make the velocity of motion of the gas subject to the action of the wave, with a drop from the initial to the sought pressure, to be also the same on both sides of the special discontinuity.

So far we have disregarded the dissipative quantities -- friction, heat conduction, and diffusion. These quantities, in combination with those available, can yield a new quantity of dimensions of length. As applied to our problem, they yield the widths of the discontinuities.

In the case of a shock wave, account of the friction and of the heat conduction, which is essential in principle for a description of the growth in the entropy, leads according to Becker to a finite and constant width of the wave front, on the order of the mean free path of the molecules in gas. This width is small compared with the distance covered by the shock wave. The dissipative quantities do not exert an essential influence on a rarefaction wave, in view of the small gradients.

For the special kind of discontinuity, dimensionality considerations lead to a width of discontinuity ξ, satisfying in order of magnitude the following relation:

$$\xi/l \simeq \sqrt{\lambda/l},$$

where l — distance which the compression or rarefaction wave covers within a given time, and λ is the mean free path of the molecules. As soon as the discontinuity is shifted by a macroscopic distance, its width will be considerably less than this distance.

Everything said above allows us to neglect dissipative quantities, as long as we do not deal with microscopic details of the construction of the discontinuities.

The structure of the rarefaction wave [Eqs. (1 — 3)] was investigated by more general and accordingly more complicated methods by Riemann [1]. The equations of a shock wave (5) — (7) were derived by Riemann in a somewhat different form, and were corrected by Hugoniot [2] and by Rayleigh [3]. The theory of propagation of arbitrary discontinuity, which includes the formation of the discontinuity of the special kind, was already constructed by Hugoniot [2], was known to Crussard [4], and is mentioned by Hadamard [5]. It was subsequently forgotten, however. Thus, for example, it is quite surprising that Weber [6] did not know of it. Nor was it known to Becker [7] for he, considering the discontinuity which results from cumulation of adiabatic compression waves, writes: "It is still unknown what takes place when the slope of the rise becomes infinite after a given time ... " i.e., when a discontinuity takes place. A solution of this problem by Becker is given below.

The propagation of an arbitrary discontinuity was considered

fully rigorously, with an analysis of the cases that can occur, by Kotchine [8]. With this, we conclude the exposition of the general theory, without making any claims for novel results, and proceed to specific problems.

Problem 1. Two gases at rest (Fig. 3) are separated by partition A, so that $P > P_0$. It is required to determine what takes place if the partition A is suddenly removed.

For small discontinuities, when $P/P_0 = 1 + \beta$, where $\beta << 1$, the problem can be solved analytically, using the well known condition that the velocities of motions of the gases must be equal on the boundary between them.

An approximate solution, accurate to second order of smallness, is obtained by the result known from acoustics

$$\frac{P - P_s}{P_s - P_0} = \frac{C\varrho_0}{C_0\varrho}, \tag{8}$$

where P_s is the pressure in the shock wave, travelling in gas I, $\varrho = 1/v$, $\varrho_0 = 1/V_0$. Eq. (8) can be rewritten as follows:

$$\frac{P - P_s}{P_s - P_0} = \frac{kC_0}{k_0 C} \quad or \quad \frac{P_s - P_0}{P - P_s} = \frac{k_0 C}{kC_0}. \tag{8a}$$

If the same gas at the same temperature exists on both sides of the plane A, then $(P_s - P_0/(P - P_s) = 1$. This last equality states that passing through gas I will be a shock wave with a pressure drop between the wave and the fresh gas, $P_s - P_0$, equal to half the

pressure drop in the discontinuity, $1/2(P - P_0)$. Travelling through gas II will be a rarefaction wave with the same pressure drop as in the shock wave.

The pressure in the occurring shock wave depends essentially on the ratio of the velocities of sound and the polytropic indices of adiabatic expansion in both gases.

If gas II is hydrogen, and gas I is air, then under idential initial temperatures, the ratio (8a) increases to four, i.e., in gas I (air), at an equal initial pressure drop, a considerably stronger shock wave is produced.

For finite discontinuities, in view of the impossibility of obtaining an analytical solution, the problem must be solved by successive approximations. Fig. 4 shows the distribution in space of the value of P and T after a certain definite time t lapsed since the occurrence of the discontinuity, for the case when on both sides of plane A there is air at an initial temperature of 20° C and a pressure ratio $P/P_0 = 100$. Fig. 5 shows an analogous diagram, the only difference being that gas II is hydrogen. The figures show that two waves are produced in the gas, travelling in different directions from the separation boundary. The discontinuity in density and temperature is a discontinuity of a special kind (plane A), which is stationary relative to the gas, and moves with the same velocity as the latter. Fig. 6 shows graphically the calculated dependence of

the pressure and temperature in the shock wave in air (gas I) at an initial temperature 20° C on the ratio of pressures at the instant of occurrence of the discontinuity. Gas II is taken to be air (curves B) and hydrogen (curves H) for the same initial temperature 20° C.

Vieille [9] investigated experimentally the propagation of the wave occurring upon rupture of a celluloid partition, dividing air at a pressure of 29 atm from air at the same temperature but with a pressure of 1 atm. He established that after the rupture of the partition, a wave with a pressure of 3.7 atm is produced, with a speed of propagation 600 meters per second. Crussard [4] has shown that the connection between the speed of propagation and the pressure in this wave is close to the connection existing in a shock wave. Our calculations, as can be verified from Fig. 6, give for the case realised by Vieille nearly the same values, 4.2 atm and 640 meters per second respectively. This indicates that the losses played a small role under the experimental conditions of Vieille.

Figs. 5 and 6 demonstrate clearly that if the gas with higher pressure is hydrogen, then higher pressures and temperatures are developed in the shock wave produced in the air than in the case of equal gases. This may explain the sometimes observed self-ignition of hydrogen upon rupture of hydrogen reservoirs or sudden

escape of hydrogen from them.

If the hydrogen is at a pressure of 150 atm, then the removal of the partition between it and the air, which is atmospheric pressure, leads at an initial temperature of 20° C to the formation of a shock wave in air, with temperature of approximately 1480 °C. Under practical conditions this temperature, generally speaking, will differ from the calculated one. In the case when the hydrogen flask bursts in an open space, or if the hydrogen escapes from it into a large free volume, the temperature will be lower than calculated, but it may nevertheless be sufficient to ignite the hydrogen on its boundary with the air. On the other hand, if the hydrogen is released into a limited volume or if obstacles exist on the path of the gas stream, it is theoretically possible for temperatures to arise greater than those calculated here, owing to the multiple reflection of the shock wave. In the limit, the compression by means of a large number of waves or small amplitude leads to a change in temperature in accordance with the adiabatic equations of Poisson.

The possible mechanism proposed for self-ignition of hydrogen does not exclude, naturally, other probable causes of flashes. It does make it possible, however, to explain self-ignition of hydrogen under certain conditions, when no other gases ignite, by using its distinguishing physical properties, primarily the low density, which

causes the aforementioned effects with shock waves. One must indicate simultaneously still another property of hydrogen, which greatly increases its explosiveness -- its ability to ignite with exceedingly short delay. Incidentally, this property increases the probability of ignition of hydrogen in the aforementioned shock waves.

Problem 2. We consider the propagation of a discontinuity produced when a large number of compression waves, the pressure drop in each is infinitesimal, propagating one after the other, combine in a single plane. In other words, we consider a discontinuity occurring upon cumulation of adiabatic compression in a single plane.

The appearance of such a discontinuity is related to the occurrence of a detonation wave in the gas, and the remark by Becker, given above, pertains to this case.

During the pre-detonation period, compression waves that follow one another are produced in a closed tube as a result of an accelerating compression in fresh gas. As follows from elementary considerations, each succeeding wave moves with a greater velocity than the preceding one. The forward wave is overtaken by the succeeding ones, and a discontinuity in the state of the gas is produced. Generally speaking, only in one particular case, which will be considered below, do all the waves reach a single plane at the same instant. This occurs, as can be readily shown for an ideal diatomic gas, if the distribution of pressure over the coordinate

satisfies the following equation:

$$\Pi = (1 + x)^{7}, \qquad (9)$$

where Π is the ratio of the pressure at a point located at a dimensionless distance x from the leading edge of the wave, to the pressure of the fresh mixture, through which the first compression wave propagates. Fig. 7 shows a plot of such a distribution. This distribution narrows down with time, remaining similar to itself, until a discontinuity in the state takes place at the plane A, together with a discontinuity in the speed of motion of the gas. As was established by Becker [7], further propagation of the discontinuity as a whole, in which the equations of the shock wave (5) — (7) are not satisfied, is impossible. What will happen to this discontinuity subsequently?

We note that gas II represents in this problem (Fig. 8) gas I, which has been adiabatically compressed to a pressure P. The velocity U can be calculated from formula (5), since such a cumulation wave of compression, of which the discontinuity is made up, can be considered as a time inversion (the reversal of the signs of x and U in the equations) of a rarefaction wave.

Let us consider the problem for small discontinuities, when $P/P_0 = 1 + p$, where $p \ll 1$. Expansion of the velocity of motion of the gas in powers of the parameter $p = P/P_0 - 1$, in the case of an ideal diatomic gas, accurate to third-order quantities, yields for

the shock wave:

$$U/C_0 = {}^5/_7 \left(p - {}^3/_7\, p^2 + {}^{27}/_{98}\, p^3 + \ldots\right) \tag{10}$$

and for the adiabatic-compression wave

$$U/C_0 = {}^5/_7 \left(p - {}^3/_7\, p^2 + {}^{26}/_{98}\, p^3 + \ldots\right). \tag{11}$$

Eqs. (10) and (11) show that the shock wave differs from the adiabatic only in quantities of third-order of smallness. Consequently, in the limiting case of small discontinuities, only one shock wave is produced in plane A (Fig. 7), propagating along gas I. The same equations show that in the case of a finite discontinuity, there is produced in addition to the shock wave travelling in gas I, a rarefaction wave travelling through gas II is produced at the plane A.

Fig. 9 shows the distribution of pressures and temperatures in air after some definite time, with a pressure ratio $P/P_0 = 50$ at the instant of occurrence of the discontinuity, and at initial temperature of gas I of 20° C. This distribution has been calculated by successive approximations. Fig. 10 shows the dependence of the pressure and temperature in the shock wave in air at the same initial temperature on the ratio of pressures on both sides of the discontinuity plane at the instant of its occurrence.

The diagrams of Fig. 9 and 10 show that a shock wave is always produced, with a pressure less than the pressure of adiabatically-compressed gas in the discontinuity. Nevertheless, the temperature

in the shock wave increases sharply compared with the temperature of the adiabatically-compressed gas. This usually /10/ explains the frequently observed occurrence of detonation at a certain distance ahead of the front of the plane.

It must be emphasized that the calculations given above can pertain only to a shock wave which ignites a gas mixture, producing a detonation. They do not give the velocities and the pressures of the detonation of the ionic wave itself, which depend essentially only on the thermal effect of the combustion reaction in the detonation wave.

3. Conclusions

1. A theory was developed for the propagation of an arbitrary discontinuity in the gas.

2. Two problems, which deal with ignition of hydrogen and the occurrence of detonation, are solved quantitatively.

Leningrad, Institute of Chemical Physics
Academy of Sciences, USSR.
Laboratory of Gas Combustion

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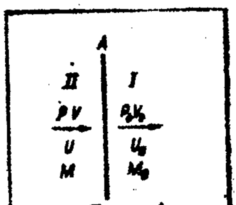

Fig. 1.

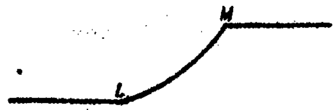

Fig. 2.

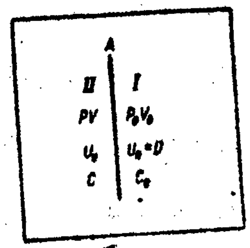

Fig. 3.

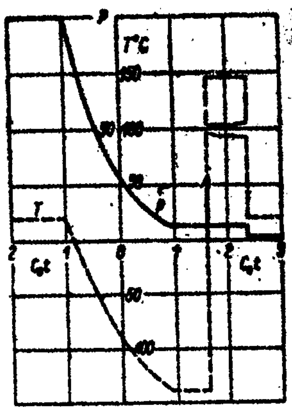

Fig. 4.

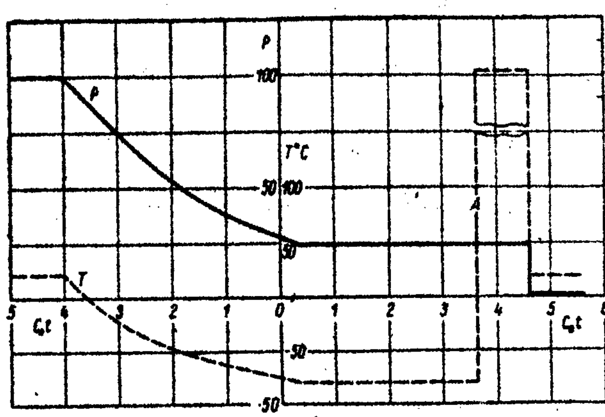

Fig. 5.

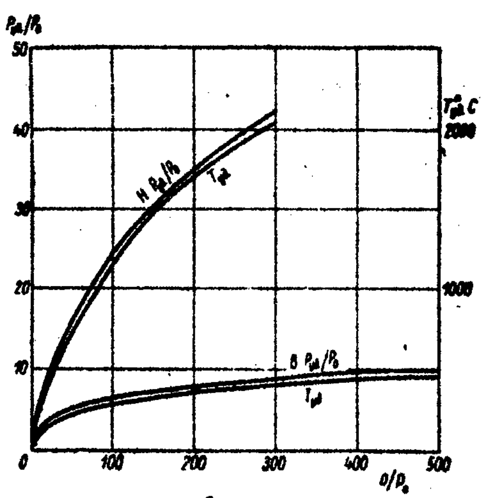

Fig. 6.

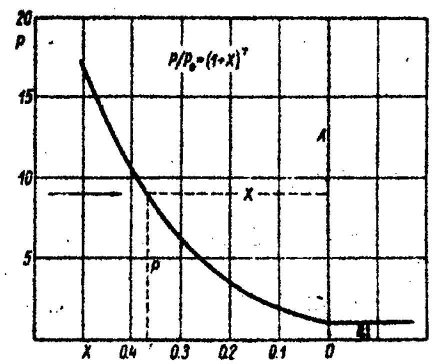

Fig. 7.

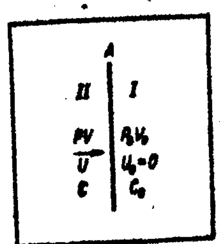

Fig. 8.

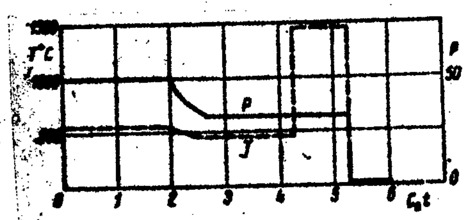

Fig. 9.

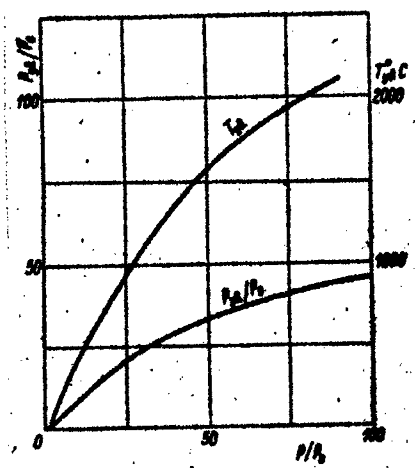

Fig. 10.

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